Introducing Computational Science in the Curriculum – Part 4

Steven I. Gordon
Senior Director of Education and Client Services
Ohio Supercomputer Center
sgordon@osc.edu

Completing the Competencies

- Growth and Decline
- Several discussion topics
  - Statistical concepts
  - Accuracy and precision
  - Verification and Validation
- Final Projects
  - General nature of the projects
  - Examples
- Final discussion

Growth and Decline

- Several possible exercises
  - Exponential growth or decline
    - Compound interest
    - Radioactive decay
  - Constrained growth
    - Population dynamics
- Will work through the population dynamics example

Problems with Unconstrained Growth

- Physical, ecological, and human systems are limited by constraints
  - Availability of energy and resources
  - Capacity constraints
- Instability caused when critical limits reached
  - Bridge collapse when vibration from high winds added to traffic
  - Steel at high temperature begins to bend and then eventually liquifies

System Stability and Feedback

- Natural environment limits
  - Sometimes defined as carrying capacity – the amount of change that can be absorbed without causing system collapse
- Both natural and manmade systems regulated through feedback
  - Negative feedback – a signal which causes the system to change in the opposite direction
    - E.G. Furnace and thermostat
    - Limited food supply reduces population growth

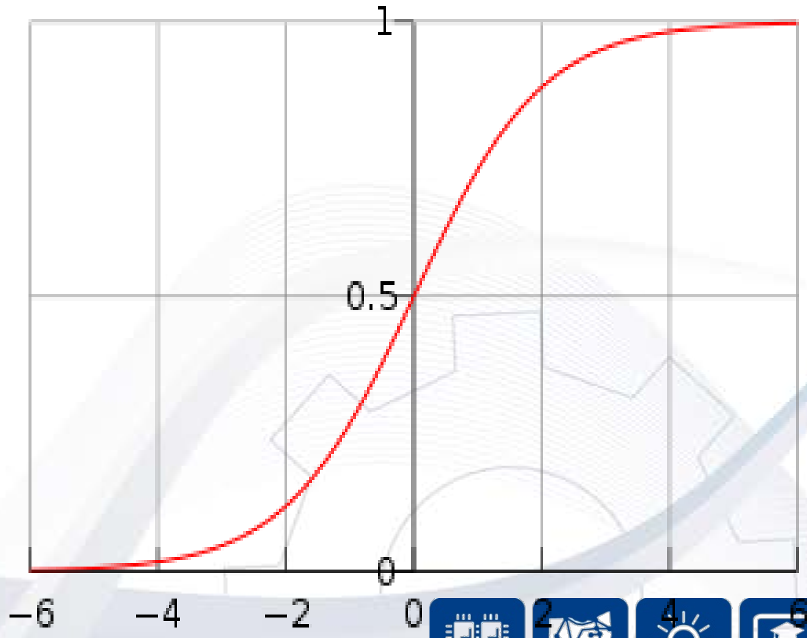
Models and Constraints

- Several modeling approaches
- Insert a lower and/or upper limit for variation
  - Works well for physical systems and some chemical characteristics
  - Examples
    - Dissolved oxygen in water – lower limit of zero and upper limit of 14.6 parts per million
    - Elevation – must be zero at earth's surface
    - Changes of state for physical substances – steel, water, nitrogen

Mathematical Constraints

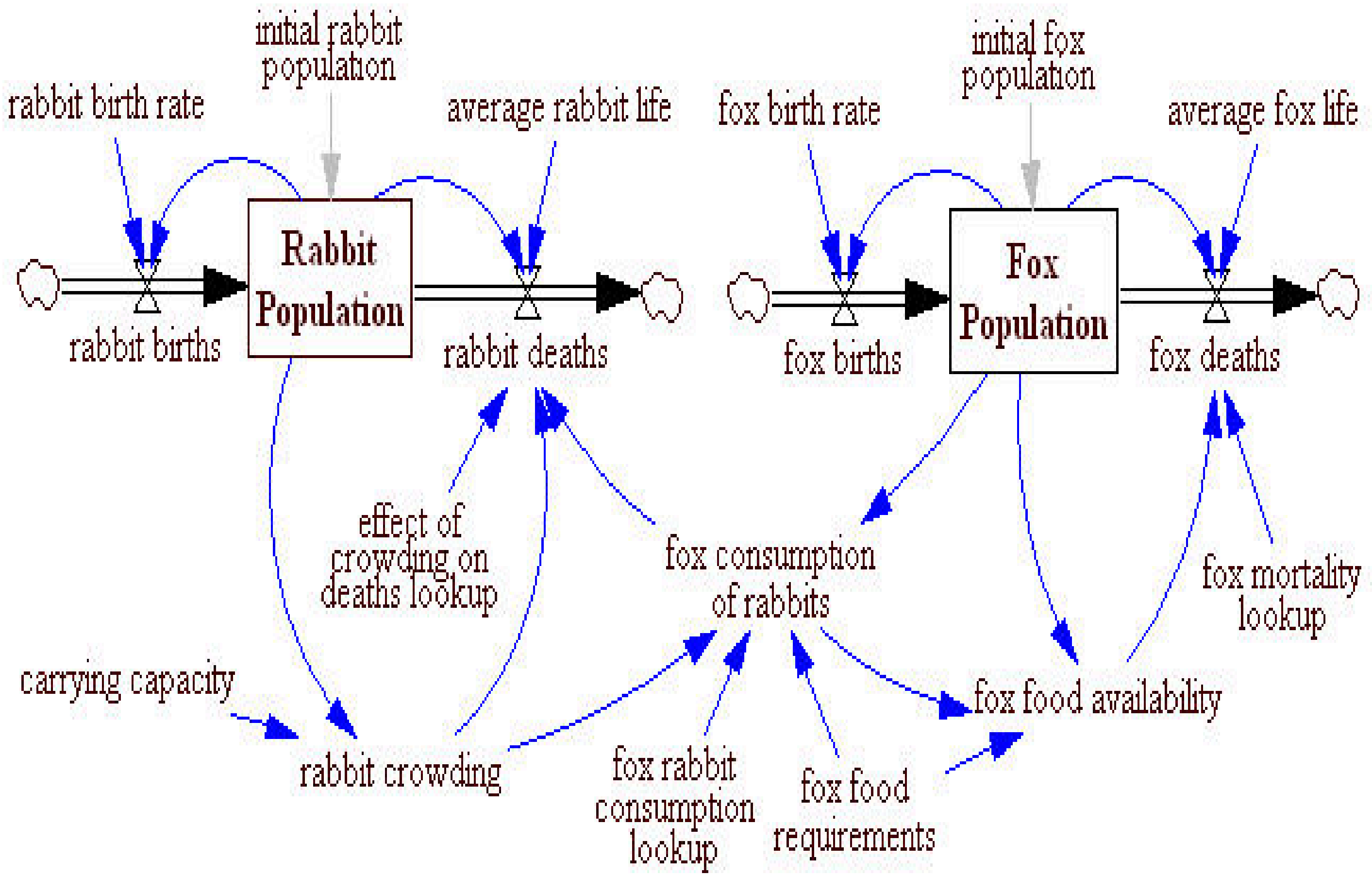
- Use mathematical functions which reflect changes in behavior and approach limits
- Logistic function

$$P(t) = \frac{1}{1+e^{-t}}$$



Explicit Modeling of Negative Feedback

- Add conditions which produce negative feedback in growth or decay
  - Population growth example
    - Changes to birth rates in response to limits of food supply
    - Increase in death rates from disease or competition
    - Impacts of crowding
    - In-breeding of population


initial rabbit population
rabbit birth rate
average rabbit life
fox birth rate
initial fox population
average fox life
Rabbit Population
rabbit births
rabbit deaths
Fox Population
fox births
fox deaths
effect of crowding on deaths lookup
fox consumption of rabbits
fox mortality lookup
carrying capacity
fox food availability
rabbit crowding
fox rabbit consumption lookup
fox food requirements

Classic Population Dynamics Model Example

- Open constrained_eg.pdf
- Examine codes
- Run code
- Discussion of modeling principles

Discussion Topics

- Not enough time to go through all other exercises
- Abridged discussion to identify aspects that complete the competencies

Statistical Concepts

- Correlation
  - Correlation coefficients
- Simple regression
  - Goodness of fit
  - Coefficient of determination
- Non-linear functions
  - Goodness of fit
- Connect later with model validation discussion

Accuracy and Precision

- Discussion of errors associated with computational models
  - Rounding and truncation errors
  - As an example open SimpleGlitches.xls
  - Implications for modeling

Verification and Validation

- Verification – determination that a program was constructed by the rules
  - Did we build the system right?
  - E.G. mathematical proof and software testing
- Validation – determination that program correctly predicts the state of the system
  - Did we build the right system?
  - Do the results approximate the real world?

Verification of Models

- Compare the computed results to a few analytically solved problems
  – Should get acceptably near the same answer
- Check the algorithm used by MATLAB or other program if possible
- Compare with other models or methods

Validation

- Carefully define the model assumptions and what those mean for the circumstances where the model will be valid
- Make a statistical comparison with empirical data from laboratory or testing results
- Define the range of the validity for which the model is tested
  - Implications of extreme, untested conditions
  - E.G. fit the wrong curve

Completing the Competencies

- Final project
  - Individual or group project using all of the accumulated programming and modeling principles
  - Start with a partially built model
  - Resources describing the underlying system and references to related models
  - Choose several new functions that relax model assumptions
  - Write and use the code to simulate system behavior
  - Make an oral and written presentation of results

Example Final Projects

- Parachute project
  - Simulate skydiver jumping from stationary platform
  - Acceleration due to gravity
  - Drag of the parachute
- Sewage project
  - Simulate the impact of sewage disposal on dissolved oxygen in a stream
  - Classic model of organic waste decomposition
  - Data from a real site to provide some measure of validation
- Take a few minutes to look over one of the examples

Questions and Discussion